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**COMPUTER PROGRAM FOR CALCULATING
PRESSURE-BROADENED RAMAN SPECTRA
FOR MOLECULAR NITROGEN AND OXYGEN**

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COMPUTER PROGRAM FOR CALCULATING PRESSURE-BROADENED RAMAN SPECTRA FOR MOLECULAR NITROGEN AND OXYGEN

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SUMMARY

A computer program is given for calculating the rotational Raman spectra for molecular nitrogen and oxygen. Provision is made for pressure broadening. Several sample results at various pressures and temperatures are shown. The relative heights of some of the lines are affected by pressure broadening, and in nitrogen the odd- j lines are most affected. For instance, the $j = 5$ anti-Stokes line increases about 15 percent relative to the $j = 6$ Stokes line for a change in pressure from 1 to 40 atmospheres, while the $j = 6$ anti-Stokes line shows no change.

INTRODUCTION

In the development of gas turbine engines, there has been a continuing goal to further increase turbine inlet temperature and thereby increase engine performance. The measurement of gas temperatures in the region of the turbine inlet and combustor exit is required to see that the combustor generates the right temperature profile as well as temperature level. Traditionally, these temperature measurements have been made with thermocouples. Presently, however, no thermocouple is available which will withstand the high temperatures and pressures (up to 2400 K and 40 atm) predicted for future turbine and combustor development.

Other methods, such as cooled immersion probes and gas analysis, have been considered as alternative solutions for making high gas temperature measurements, but as yet none have been used on a routine basis. Another method of current interest is a remote-sensing light-scattering technique utilizing Raman scattering. The Raman scattering technique is attractive in that it can be used to focus remotely on a small volume in a gas stream and extract information associated with local gas density, composition, and temperature.

Over the last few years several groups have been conducting development work on this technique (refs. 1 to 5), and, in at least one case, the technique has been applied to the measurement of jet engine exhaust temperatures up to 955 K (ref. 6).

Some of the problems associated with the use of Raman scattering in measuring temperature in jet engine exhaust gases are fluorescence, ambient light background, interference of various species of gas, and pressure broadening.

This investigation was conducted to extend the results found in reference 2 to produce a computer program for computing the Raman spectra which includes the effects of pressure broadening. This program can be used to predict the extent of pressure broadening associated with temperature measurements at elevated pressures.

THEORY

The theory of rotational Raman scattering and line broadening is discussed in references 1 and 2, so that only a relatively brief outline is given in this section.

When a beam of light, from a laser, for example, is scattered from a molecular system, most of the light is scattered with no change in wave number (the wave number is the inverse of the wavelength). This is called Rayleigh scattering. Some of the scattering molecules, however, are induced into undergoing a change of energy level by the light beam, and the scattered light has a wave number different from that of the incident light. This is called Raman scattering. If the molecule undergoes a transition to an energy state lower than it originally had, the wave number of the scattered light is increased (anti-Stokes scattering); conversely, if the molecule undergoes a transition to a higher energy state, the wave number of the scattered light is decreased (Stokes scattering). Because the molecular energy levels are quantized (discrete), the wave number shifts are also discrete, and the spectrum of the scattered light consists of the unshifted Rayleigh line and a series of lines on either side of it, the Raman lines. The magnitude of the frequency shifts and the relative intensities of the various lines depend on what type of molecule is involved and on the temperature.

The scattered light is not observed as a series of perfectly sharp lines, but as lines which are spread out, or broadened. The broadening has a variety of causes, among which are the fact that neither the light source nor the detector is perfectly monochromatic and the fact that the molecules are in motion rather than being at rest. Since the broadening depends on both the temperature and pressure of the gas, it must be taken into account if Raman scattering is to be used as a tool for measuring the temperature of high-pressure gases.

If the Raman scattered light from a molecule has an intensity I_j , where j is the quantum number associated with a particular line, the broadening of that line is described by writing

$$I_j(\nu) = I_j S(\nu, \nu_j) \quad (1)$$

That is, the intensity at wave number ν due to the line located at ν_j and having an intensity I_j is found by multiplying I_j by the factor $S(\nu, \nu_j)$. This is shown in figure 1. The factor $S(\nu, \nu_j)$ is called the normalized shape function (ref. 2). (Symbols are defined in appendix A.)

For a series of spectral lines, the intensity at ν is just the sum of the intensities due to each line

$$I(\nu) = \sum_j I_j(\nu) = \sum_j I_j S(\nu, \nu_j) \quad (2)$$

The Raman spectrum is the intensity at each value of ν , so the problem of calculating the spectrum reduces to calculating the line intensities I_j and the normalized shape function $S(\nu, \nu_j)$. The shape function $S(\nu, \nu_j)$ is normalized to unit area in order to satisfy the requirement of conservation of energy. The total intensity of the broadened lines over all wave numbers is

$$\int_{-\infty}^{\infty} I(\nu) d\nu = \sum_j I_j \int_{-\infty}^{\infty} S(\nu, \nu_j) d\nu = \sum_j I_j$$

which is the total intensity of all the unbroadened lines.

The Raman lines on the low-wave-number side of a Rayleigh line are called the Stokes lines, and for the rotational scattering from the diatomic nitrogen and oxygen molecules (N_2 and O_2) considered in this report the line intensities are given by references 2 and 7 as

$$I_j^{(S)} = C_j \frac{(j+1)(j+2)}{2j+3} \frac{\theta}{T} (\nu_0 - \Delta\nu_j)^4 e^{-\theta j(j+1)/T} \quad j = 0, 1, 2, 3, \dots \quad (3)$$

The lines on the other side of the Rayleigh line are called the anti-Stokes lines, and their intensities are given by

$$I_j^{(AS)} = C_j \frac{(j+1)(j+2)}{2j+3} \frac{\theta}{T} (\nu_0 + \Delta\nu_j)^4 e^{-\theta(j+2)(j+3)/T} \quad j = 0, 1, 2, 3, \dots \quad (4)$$

where C_j contains other factors, such as nuclear spin. The spin causes the intensity of every other N_2 line to be reduced by 50 percent and causes every other O_2 line to be absent. The wave number ν_0 is the wave number of the laser, and

$$\Delta \nu_j = \frac{4k\theta}{hc} \left(j + \frac{3}{2} \right) \quad (5)$$

is the wave number shift. The lines are located at

$$\nu_j = \nu_0 \pm \Delta \nu_j \quad (6)$$

The constant θ is called the rotational characteristic temperature of the molecule.

Line broadening is due to the Doppler profile in the laser, combined natural and pressure broadening in the molecular gas, and instrument distortion (ref. 2). The profile of the laser line is given by a Gaussian function (refs. 8 and 9)

$$S_L(\nu, \nu_0) = \frac{2\sqrt{\ln 2}}{\sqrt{\pi} R_L} e^{-\left(4 \ln 2 / R_L^2\right) (\nu - \nu_0)^2} \quad (7)$$

and the natural-pressure broadening by a Lorentz profile (ref. 10).

$$S_R(\nu, \nu') = \frac{\frac{R_R}{2}}{\pi \left[(\nu - \nu')^2 + \left(\frac{R_R}{2} \right)^2 \right]} \quad (8)$$

The combined effect of the Doppler profile and natural-pressure broadening is given by the Voigt broadening function, which is the convolution of S_L and S_R :

$$S_V(\nu, \nu_j) = \int_{-\infty}^{\infty} S_L(\nu', \nu_j) S_R(\nu, \nu') d\nu' = \frac{\sqrt{\ln 2} R_R}{\pi^{3/2} R_L} \int_{-\infty}^{\infty} \frac{e^{-\left(4 \ln 2 / R_L^2\right) (\nu' - \nu_j)^2}}{(\nu - \nu')^2 + \left(\frac{R_R}{2} \right)^2} d\nu' \quad (9)$$

Note that the two broadening functions S_L and S_R are normalized to unit area. For this reason, S_V is also normalized to unit area:

$$\begin{aligned}
\int_{-\infty}^{\infty} S_V(\nu, \nu_j) d\nu &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} S_L(\nu', \nu_j) S_R(\nu', \nu) d\nu' d\nu \\
&= \int_{-\infty}^{\infty} S_L(\nu', \nu_j) \int_{-\infty}^{\infty} S_R(\nu', \nu) d\nu d\nu' \\
&= \int_{-\infty}^{\infty} S_L(\nu', \nu_j) d\nu' = 1
\end{aligned}$$

The two numbers R_L and R_R are called, respectively, the laser and Raman bandwidths and give the width of a profile when the height is reduced to one-half of the peak value, as shown in figures 2 and 3. The bandwidth R_L is constant, but the bandwidth R_R is not. It varies with temperature, pressure, and the quantum number j . The form of the variation, deduced from the data in references 11 and 12, is

$$R_R = \sqrt{\frac{T_0}{T}} (jA + B)P \quad (10)$$

where T_0 is a reference temperature, T is the gas temperature, and P is the gas pressure. The constants A , B , and T_0 are fitted to experimental data measured by using gases of known temperature and pressure.

The behavior of line broadening due to the detecting instrument is given by the slit function (ref. 13)

$$S_S(\nu, \nu_S) = \frac{2\sqrt{\ln 2}}{\sqrt{\pi} R_S} e^{-\left(4 \ln 2 / R_S^2\right)(\nu - \nu_S)^2} \quad (11)$$

Finally, the combined effect of all the broadening is the convolution of the Voight and slit functions to yield the overall shape function

$$S(\nu, \nu_j) = \int_{-\infty}^{\infty} S_S(\nu, \nu') S_V(\nu', \nu_j) d\nu' = \frac{2\sqrt{\ln 2}}{\sqrt{\pi} R_S} \int_{-\infty}^{\infty} e^{-\left(4 \ln 2 / R_S^2\right)(\nu' - \nu)^2} \frac{\sqrt{\ln 2} R_R}{\pi^{3/2} R_L} \int_{-\infty}^{\infty} \frac{e^{-\left(4 \ln 2 / R_L^2\right)(\nu'' - \nu_j)^2}}{(\nu'' - \nu')^2 + \left(\frac{R_R}{2}\right)^2} d\nu'' d\nu' \quad (12)$$

The shape function is also normalized to unit area, as explained previously.

In principle, the spectrum can now be calculated by substituting I_j from equation (3) or (4) and $S(\nu, \nu_j)$ from equation (12) into equation (2). Unfortunately, the integrals in equation (12) cannot be evaluated analytically, but must be evaluated numerically.

The inner integral in equation (12), the Voigt integral, can be put into another form, for which numerical solutions now exist. Let

$$\alpha = \frac{2\sqrt{\ln 2}}{R_L} \quad \beta = \frac{R_R}{2}$$

so that

$$S_V(\nu', \nu_j) = \alpha\pi^{-3/2} \int_{-\infty}^{\infty} \frac{e^{-\alpha^2(\nu'' - \nu_j)^2}}{(\nu'' - \nu')^2 + \beta^2} d\nu'' \quad (13)$$

With the change of variables

$$\left. \begin{aligned} y &= \frac{\nu'' - \nu'}{\beta} \\ x &= \frac{\nu_j - \nu'}{\beta} \end{aligned} \right\} \quad (14)$$

The result is

$$S_V(\nu', \nu_j) = \alpha\pi^{-3/2} \int_{-\infty}^{\infty} \frac{e^{-\alpha^2\beta^2(y-x)^2}}{1 + y^2} dy \quad (15)$$

Now let

$$\Theta = 2\alpha\beta = 2\sqrt{\ln 2} \frac{R_R}{R_L} \quad (16)$$

The Voigt integral may be expressed in terms of the first Doppler broadening integral (ref. 14)

$$S_V(\nu', \nu_j) = \alpha \beta \pi^{-3/2} \left[\frac{2\sqrt{\pi}}{\Theta} \psi(x, \Theta) \right] = \frac{2}{\pi R_R} \psi(x, \Theta) \quad (17)$$

and aside from a constant factor independent of j , the shape function becomes

$$S(\nu, \nu_j) = \frac{1}{R_R} \int_{-\infty}^{\infty} e^{-\left(4 \ln 2 / R_S^2\right)(\nu' - \nu)^2} \psi(x, \Theta) d\nu' \quad (18)$$

The j -independent part of the normalization constant is dropped because only the relative peak heights are of concern.

Since reference 14 supplies a computer program for numerically evaluating $\psi(x, \Theta)$ (listed in appendixes B and C as PSIPHI), the shape function can now be found numerically as soon as realistic limits of integration are found to replace the infinite limits shown in equation (18). The details of finding these limits are given in appendix D.

DISCUSSION OF RESULTS

Eight sample results are included in figures 4 to 11. These are results for N_2 and O_2 at 1, 20, and 40 atmospheres and 300 K, for N_2 at 1 atmosphere and 1100 K, and for N_2 at 19.4 atmospheres and 300 K. The results are normalized so that the highest peak has the value of 10. The laser line was taken as 5145×10^{-10} meter (5145 Å) (Ar^+ laser), and the spectra were calculated on a 30×10^{-10} -meter (30-Å) interval on either side of the laser line (60×10^{-10} m (60 Å) for N_2 at 1 atm and 1100 K). Note that the calculated spectra do not include the Rayleigh line. The following values were used for the constants:

Molecular rotational characteristic temperature θ , K

| | |
|---|---------|
| For nitrogen | 2.862 |
| For oxygen | 2.065 |
| Laser bandwidth, R_L , cm^{-1} | 0.166 |
| Slit bandwidth, R_S , cm^{-1} | 3.31 |
| Pressure-broadening constant, A , cm^{-1}/atm | -0.0025 |
| Pressure-broadening constant, B , cm^{-1}/atm | +0.091 |
| Reference temperature for R_R , T_0 , K | 303 |

The values for A and B , the pressure-broadening constants, and T_0 , the reference temperature, were obtained from the data given in references 11 and 12. The same values were used for both nitrogen and oxygen. A Raman spectrum for N_2 at 19.4 atmospheres and 300 K measured in a high-pressure furnace at the Lewis Research Center is included in figure 11 for comparison. The agreement between it and the calculated spectrum shown in figure 11 is satisfactory, although better values for A and B have yet to be determined. The fact that the locations of the higher j lines are different in the two spectra indicates that there is also a small error in θ .

As can be seen, the effect of pressure broadening is considerable, at least on the odd- j lines. For instance, the $j = 5$ anti-Stokes line in N_2 increases in relative height about 15 percent as the gas pressure is increased from 1 to 40 atmospheres. The $j = 6$ anti-Stokes line does not increase at all. The odd- j lines are more affected by broadening because they are between two tall lines, and the even- j lines are between two short lines.

Increasing the temperature has the effect of increasing the height of all the lines and shifting the highest intensity line toward higher j values. At 300 K, the highest line is the $j = 6$ Stokes line, and at 1100 K the highest line is the $j = 12$ Stokes line.

CONCLUDING REMARKS

A computer program is presented which is capable of calculating the rotational Raman spectrum of either N_2 or O_2 and which includes the effect of pressure broadening. Although a general spectrum can be computed, the best method of using these calculations to determine the temperature of a high-pressure gas has not yet been determined. Nevertheless, the sample calculations (figs. 4 to 11) show that the effects of pressure broadening are not negligible for the pressures of interest in future combustor applications (up to 40 atm).

Lewis Research Center,
National Aeronautics and Space Administration,
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505-04.

APPENDIX A

SYMBOLS

| | |
|---------------------|---|
| A, B | pressure-broadening constants, $\text{cm}^{-1}/\text{atm}$ |
| C_j | spin factor for unbroadened lines |
| c | speed of light |
| h | Plank constant |
| $I(\nu)$ | intensity of broadened line at wave number ν |
| I_j | intensity of unbroadened line, $(W/\text{cm}^2)/\text{cm}^{-1}$ |
| $I_j^{(\text{AS})}$ | intensity of anti-Stokes line |
| $I_j^{(\text{S})}$ | intensity of Stokes line |
| $I_j(\nu)$ | intensity associated with broadening of single line |
| j | rotational quantum number |
| k | Boltzmann constant |
| P | pressure, atm |
| R_L | laser bandwidth, cm^{-1} |
| R_R | natural-pressure bandwidth |
| R_S | slit bandwidth |
| $S(\nu, \nu_j)$ | normalized broadening function |
| S_L | laser broadening function |
| S_R | natural-pressure broadening function |
| S_S | slit broadening function |
| S_V | Voight function |
| T | temperature, K |
| T_0 | reference temperature for R_R |
| x | parameter in Doppler broadening integral |
| Θ | parameter in Doppler broadening integral |
| θ | molecular rotational characteristic temperature, K |
| λ | wavelength, 0.1 nm (\AA) |
| ν | wave number, cm^{-1} |

ν_j wave number of unbroadened line
 $\Delta \nu_j$ wave number shift of j^{th} line
 ν_0 wave number of laser line
 $\psi(x, \Theta)$ first Doppler broadening integral

APPENDIX B

DESCRIPTION OF PROGRAM

The computer program is written in FORTRAN IV for use on the IBM 360.

The main program is called MAIN1. In this program, all the necessary constants are read in, and all the various parameters needed by the subprograms are calculated, as are the number and location of the rotational lines for either oxygen or nitrogen. The program uses wave numbers (cm^{-1}) in the calculations and determines the intensity $I(\nu) = \sum I_j S(\nu, \nu_j)$ at each value of ν . The value of I_j is calculated by the subroutine XNITRO.

Equation (A10) indicates that the bandwidth of $S(\nu, \nu_j)$ is roughly $\sqrt{R_V^2 + R_S^2}$, so computing time is reduced by excluding any value of ν_j (the center of the j^{th} line) which is farther than $3\sqrt{R_V^2 + R_S^2}$ from ν from the above sum. For convenience in plotting, the output is in terms of $I(\lambda)$, where λ is the wavelength in tenths of a nanometer (angstroms).

The actual calculation of $S(\nu, \nu_j)$ takes place in the function subprogram called SHPFN. There the integration limits are calculated for each value of ν . SHPFN calls the function PROD, which in turn calls the function VOIGHT, which uses subroutine PSIPHI to produce $\psi(x, \Theta)$. PROD also uses ν the function SLTFN to produce $S_S(\nu, \nu)$. The function PROD is the product of S_S and ψ . SHPFN uses the integration routine QUAD1 to integrate PROD between the limits $\nu_C \pm 3B_W$. The result is then SHPFN = $S(\nu, \nu_j)$. The slit function was made a separate subprogram so that it could easily be changed if desired. For instance, a Lorentz distribution instead of a Gaussian function could be used.

APPENDIX C

PROGRAM LISTING

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C...  MAIN1, MAIN PROGRAM FOR CALCULATING ROTATIONAL RAMAN SPECTRUM OF N2 OR O2
      COMMON/BASIC/CENTER
      COMMON/SPEC/RATIO, IHALF, LEN, IND
      COMMON/RAM/RR, RL, RS
      COMMON/VPARAM/THET
      COMMON/SLPARAM/CON
      COMMON/SPARAM/RVSQ, RSSQC, DENOM, THREEB
      DIMENSION RSBR (100), RSBVSQ (100), THRB (100), DENM (100), CTOFF (100), THT (100)
      DIMENSION DELNU (100), DNU (2)
      DIMENSION ANG (1000), TENS (1000), COUNT (1000)
      INDEX=1
1     WRITE (6, 101)
101    FORMAT (1H0' STEP 1-ROTATIONAL RAMAN SPECTRUM OF NITROGEN(ENTER 1.) OR OXYGEN(ENTER 2.)')
      READ (5, 201) EL
      LEN=IFIX (EL)
2     WRITE (6, 102)
102    FORMAT (1H0' STEP 2-WHAT IS THE ROTATIONAL CHARACTERISTIC TEMP. (DEG. K) ?')
      READ (5, 201) THETA
201    FORMAT (F10.2)
      C1=2.7808*THETA
3     WRITE (6, 103)
103    FORMAT (1H0' STEP 3-ENTER THE LASER AND SLIT BANDWIDTHS (INV. CM.)')
      READ (5, 201) RL
      READ (5, 201) RS
      RSSQ=RS*RS
      CON=2.7725887/RSSQ
      THE=1.6651092/RL
4     WRITE (6, 104)
104    FORMAT (1H0' STEP 4-WHAT IS THE WAVELENGTH OF THE LASER LINE (ANGSTROMS) ?')
      READ (5, 201) ALAMO
5     WRITE (6, 105)
105    FORMAT (1H0' STEP 5-OVER WHAT RANGE (ANGSTROMS) ON EITHER SIDE OF THE CENTER IS THE INTENSITY TO BE CALCULATED ?')
      READ (5, 201) ALMRNG
      ALMMIN=ALAMO-ALMRNG
      ALMMAX=ALAMO+ALMRNG
      XNUO=1.E+08/ALAMO
      XNUMAX=1.E+08/ALMMIN
      XNUMIN=1.E+08/ALMMAX
      XNURNG=XNUMAX - XNUO
C...  CALCULATE THE NUMBER OF ROTATIONAL LINES
      BJ=AINT (XNURNG/C1 - 1.)
      BJ=BJ+1.
      NTERM=IFIX (BJ)
6     WRITE (6, 106)
106    FORMAT (1H0' STEP 6-AT HOW MANY POINTS IN THS RANGE IS THE INTENSITY TO BE CALCULATED (500. MAX.) ?')
      READ (5, 201) PTNO
      NPTNO=IFIX (PTNO)
      DNU (1)=XNURNG/PINO
      DNU (2)=(XNUO-XNUMIN)/PTNO
7     WRITE (6, 107)
107    FORMAT (1H0' STEP 7-ENTER THE GAS TEMP. (DEG. K) AND THE GAS PRESSURE (ATM.)')
      READ (5, 201) TEMP
      READ (5, 201) PRESS
      TPFAC=SQRT (303./TEMP)*PRESS
      RATIO=THETA/TEMP
8     WRITE (6, 108)
108    FORMAT (1H0' STEP 8-ENTER THE PRESSURE BROADENING CONSTANTS, A & B')

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```

      READ(5,201) A
      READ(5,201) B
C...  CALCULATE VARIABLES WHICH DEPEND ON LINE NUMBER
      DO 1000 KL=1, NTERM
      K=KL-1
      AK=FLOAT(K)
C...  CALCULATE PRESSURE BROADENED RAMAN BANDWIDTH
      RR=TPFAC*(A*AK + B)
      RSBR(KL)=RR
      RRO2=RR/2.
C...  CALCULATE VOIGT BANDWIDTH
      RV=RRO2 + SQRT(RRO2**2 + RL**2)
      RVSQ=RV**2
      RSBVSQ(KL)=RVSQ
      THREEB=3./SQRT(1./RSSQ + 1./RVSQ)
      THRB(KL)=THREEB
      DENOM=RSSQ + RVSQ
      DENM(KL)=DENOM
      CTOFF(KL)=3.*SQRT(DENOM)
C...  CALCULATE VOIGT PARAMETER
      THET=THE*RR
      THT(KL)=THET
      DELNU(KL)=C1*(AK + 1.5)
      CENTER=XNUO + DELNU(KL)
      RSSQC=RSSQ+CENTER
1000  CCNTINUE
C...  CALCULATE SPECTRUM. IHALF = 1 IS ANTI-STOKES SIDE
      DO 4000 IHALF = 1,2
      SIGN=1.
      IF (IHALF .EQ. 2) SIGN=-1.
      DO 3000 M=1, NPTNO
      XNUU=XNUO + SIGN*FLOAT(M)*DNU(IHALF)
      L=NPTNO-M+1
      IF (IHALF .EQ. 2) L=NPTNO + M
      ANG(L)=1.E+08/XNUU
      SUM=0.
      DO 2000 I=1, NTERM
      J=I-1
      IND=2
      IF (2*(J/2) .NE. J) IND=1
C...  IND=1 IF J IS ODD, IND=2 IF J IS EVEN
      XJ=PLCAT(J)
      RR=RSBR(I)
      RVSQ=RSBVSQ(I)
      THREEB=THRB(I)
      DENOM=DENM(I)
      CUTOFF=CTOFF(I)
      THET=THT(I)
      CENTER= XNUO + SIGN*DELNU(I)
      RSSQC=RSSQ+CENTER
      TST=ABS(XNUU - CENTER)
C...  SKIP LINES WHICH ARE TOO FAR AWAY TO CONTRIBUTE & SKIP EVEN O2 LINES
      IF ( (TST .GE. CUTOFF) .OR. (LEM .EQ. 2 .AND. IND .EQ. 2) ) GO TO 2000
      CALL XNITRO(XJ,PK)
      SUM = SUM + PK*SHEFN(XNUU)/RR
2000  CONTINUE
      TENS(L)=SUM
3000  CCNTINUE
4000  CONTINUE
9     WRITE(7,110) INDEX
      IF (INDEX .NE. 1) GO TO 11
C...  INDEX=2 TELLS PLOTTING ROUTINE NO MORE DATA IS TO FOLLOW
C...  NORMALIZE & FEED INTO DATASET "DATA1" FOR PLOTTING, USING WRITE(7,...)
      NT=4*NPTNO
C...  NT IS TOTAL NO. OF POINTS, COUNTS & WAVELENGTHS, FROM BOTH SIDES OF THE SPECTRUM
      NTOT=2*NPTNO
C...  FIND LARGEST VALUE
      AMAX=TENS(1)
      DO 5000 II=2, NTOT
      IF (TENS(II) .GT. AMAX) AMAX=TENS(II)
5000  CONTINUE
C...  SCALE SO THAT LARGEST VALUE IS 10
      XNCRM=.1*AMAX

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```

        WRITE(7,110) LEM
        WRITE(7,110) NT
110    FORMAT(I4)
        WRITE(7,111) TEMP
        WRITE(7,111) PRESS
111    FORMAT(E13.6)
        DO 6000 K=1,NTOT
        COUNT(K)=TENS(K)/XNORM
C...   DATA IS FED IN SERIALLY. THE FIRST NO. IS THE HEIGHT OF THE SPECTRUM AT POINT K,COUNT(K),AND THE
C...   SECCND IS THE LOCATION OF THE POINT IN ANGSTROMS,ANG(K).
        WRITE(7,111) COUNT(K)
6000   WRITE(7,111) ANG(K)
        WRITE(6,109)
109    FORMAT(1H0'TO WHICH STEP DO YOU WISH TO RETURN?-9 GETS YOU OUT')
        READ(5,202) ML
202    FORMAT(I1)
        GO TO (1,2,3,4,5,6,7,8,10),ML
10     INDEX=2
        GO TO 9
11     STOP
        END

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```

        SUBROUTINE XNITRO(AJ,PKHT)
C...   CALCULATES PEAK HEIGHT,PKHT, FOR NITROGEN(LEM=1) & FOR OXYGEN(LEM=2) FOR ODD VALUES OF J
        COMMON/SPEC/RATIO,IHALF,LEM,IND
        COMMON/BASIC/CENTER
C...   OVERALL CONSTANT OMITTED
        C=RATIO*(AJ+1.)*(AJ+2.)*(CENTER**4)/(2.*AJ + 3.)
        IF(IHALF.EQ. 1) GO TO 1
        PKHT=C*EXP(-RATIO*AJ*(AJ+1.))
        IF(LEM.EQ. 2) RETURN
        GO TO 2
1       PKHT=C*EXP(-RATIO*(AJ+2.)*(AJ+3.))
        IF(LEM.EQ. 2) RETURN
C...   ODD J LINES ARE HALF INTENSITY FOR NITROGEN
2       IF(IND.EQ. 1) PKH1=0.5*PKHT
        RETURN
        END

```

```

        FUNCTION SHPPN(XNU)
C...   CALCULATES UNNORMALIZED SHAPE FUNCTION AT WAVE NO. XNU
        COMMON/SPARAM/RVSQ,RSSQC,DENOM,THREEB
        COMMON/WVNO/GNU
        EXTERNAL PROD
        GNU=XNU
C...   CALCULATE INTEGRATION LIMITS
        CENT=(RVSQ*XNU + RSSQC)/DENOM
        XMIN=CENT - THREEB
        XMAX=CENT + THREEB
        SHPPN=QUAD1(5,3,XMIN,XMAX,PROD)
        RETURN
        END

```

```

        FUNCTION PROD(XNP)
C...   PRODUCT FUNCTION NEEDED BY QUAD1
        COMMON/FLAG/KF
        COMMON/WVNO/GNU
        XNN=GNU
        FAC1=SLTFN(XNP,XNN)
        IF(KF.EQ. 2) GO TO 1
        PROD=FAC1*VOIGHT(XNP)
        GO TO 2
1       PROD=0.
2       RETURN
        END

```

```

        FUNCTION VOIGHT(XN)
C...   CALCULATES VOIGHT FUNCTION BY USING FIRST DOPPLER BROADENING INTEGRAL

```



```

COMMON/5AM/RR,RL,RS
COMMON/BASIC/CENTER
COMMON/VPARAM/THET
C... OVERALL CONSTANT OMITTED
X=2.*(CENTER-XN)/RR
CALL PSIPHI(X,THET,PSI,PHI)
VOIGHT=PSI
RETURN
END

FUNCTION SLTPN(X,XS)
C... GAUSSIAN SLIT FUNCTION CENTERED AT XS,BANDWIDTH RS
COMMON/SLPRAM/CCN
COMMON/FLAG/KF
ARG=CON*(X-XS)**2
IF(ARG.GE.170.) GO TO 1
SLTPN=EXP(-ARG)
KF=1
GC TO 2
1 SLTPN=0.
KF=2
2 RETURN
END

SUBROUTINE PSIPHI(XX,TT,U,V)
C... REF: B. CARRIGHT & T. SEMLER, TM X-2559
C... XX = 2.*(NU SUB J - NU)/RR
C... TT = THETA = 2.*SQRT(LN(2.))*RR/RL
C... U & V ARE FIRST AND SECOND DOPPLER BROADENING INTEGRALS
C...
C... H=1.
DIMENSION EMN(5),EN2(10)
DATA PI22/12.566371/
DATA RTPI/1.7724539/,PIH/1.5707963/
DATA PI,PI2,N/3.1415927,6.2831854,5/
DATA EMN/0.,.11709966E0,.58300489E-2,.39282561E-4,-
1 .35821059E-7/
DATA EN2/0.,.24789999,.11709966,.33549615E-1,.58300489E-2,-
2 .61448264E-3,.39282561E-4,.15231502E-5,.35820159E-7,.51095996E-9/
XD=ABS(XX)
THETA=ABS(TT)
Y=THETA/2.
X=XD*Y
C... ARE WE IN DANGER?
XTEST=X-AINT(X)
IF( (XTEST.LT..01 .OR. XTEST.GT..99) .AND. ABS(Y).LT..01) GO TO 40
IF( XD.GT.75.*SQRT(1.+1./(Y*Y)) ) GO TO 30
IF(Y.LT..001) GC TO 40
C... BEGIN SERIES SUMMATION
Y2=Y*Y
C... SET N=0 TERM
D=PI*(X*X + Y2)
SU=Y/D
SV=X/D
DO 10 I=2,N
AM=FLOAT(I-1)
XNP=X-AM
XNM=X+AM
DP=XNP*XNP + Y2
DM=XNM*XNM + Y2
SU = SU + EMN(I)*Y*(1./DP + 1./DM)
SV = SV + EMN(I)*(XNP/DP + XNM/DM)
10 CONTINUE
IF(Y.GT.PI) GC TO 20
P=2.
IF(Y.EQ.PI) P=1.
C... BEGIN POLE CONTRIBUTION
XP2=X*PI2
ARG1=Y*PI2
IF(ARG1.LE.-170.) GO TO 14
EYP2=EXP(ARG1)

```

```

14 GO TO 15
15 EYP2=0.
CONTINUE
XY2=X*Y*2.
SXY2=SIN(XY2)
CXY2=COS(XY2)
SXP2=SIN(XP2)
CXP2=COS(XP2)
ARG2=Y2 - X*X
IF (ARG2 .LE. -170.) GO TO 16
EYX=EXP(ARG2)
GO TO 17
16 EYX=0.
17 D = 1. - EYP2*(2.*CXP2 - EYP2)
SU = SU + P*EYX*( CXY2 - EYP2*(CXP2*CXY2 + SXP2*SXY2) )/D
SV = SV - P*EYX*( SXY2 + EYP2*(SXP2*CXY2 - CXP2*SXY2) )/D
20 U=SU*Y*RTPI
V=SV*THETA*RTPI
IF (XX .LT. 0.) V=-V
GO TO 50
30 F=RTPI*Y
SU = 1./((1. + XD*XD)*P)
SV=SU*XD
GO TO 20
40 CONTINUE
IF (XD .LT. 4. .AND. THETA .LE. .009) WRITE(6,101) XD,THETA
101 FORMAT(1H0'XD = 'E13.7,'THETA = 'E13.7,'FROM PSIPH')
C... THIS IS EXPANSION WITH H=0.5
Y2=Y*Y
D=PI*(X*X + Y2)
SU=Y/D
SV=X/D
DO 45 I=2,10
AM=0.5*FLOAT(I-1)
XNP=X-AM
INN=X+AM
DP=XNP*XNP + Y2
DN=INN*INN + Y2
SU = SU + EN2(I)*Y*(1./DP + 1./DN)
SV = SV + EN2(I)*(XNP/DP + INN/DN)
45 CONTINUE
SU=SU*0.5
SV=SV*0.5
IF (Y .GT. PI2) GO TO 20
P=2.
IF (Y .EQ. PI2) F=1.
XP2=X*PI22
ARG3=Y*PI22
IF (ARG3 .LE. -170.) GO TO 48
EYP2=EXP(ARG3)
GO TO 15
48 EYP2=0.
GO TO 15
50 RETURN
END

FUNCTION QUAD1(NN,NS,XI,XO,POFX)
C NUMERICAL INTEGRATION USING THE METHOD OF GAUSSIAN QUADRATURE
C NN=NO. OF POINTS/DIVISION, NN=3,4,5,...,16
C NS=NO. OF DIVISIONS INTO WHICH THE INTERVAL (XO - XI) IS DIVIDED
C XI=LOWER LIMIT OF INTEGRATION
C XO=UPPER LIMIT OF INTEGRATION
C POFX=USER SUPPLIED EXTERNAL FUNCTION SUBPROGRAM
DIMENSION C(140),A(70),H(70),AA(56),BB(56),CC(28)
REAL INTGRL
EQUIVALENCE (AA(1),C(1)),(BB(1),C(57)),(CC(1),C(113))
DATA AA/-
1 7.74596669241483E-01, 5.55555555555556E-01,-0. E-00,-
1 8.88888888888889E-01, 8.61136311594053E-01, 3.47854845137454E-01,-
1 3.39981043584856E-01, 6.52145154862546E-01, 9.06179845938664E-01,-
1 2.36926885056189E-01, 5.38469310105683E-01, 4.78628670499366E-01,-
1-0. E-00, 5.68888888888889E-01, 9.32469514203152E-01.-

```

```

1 1.71324492379170E-01, 6.61209386466265E-01, 3.60761573048139E-01,-
1 2.38619186083197E-01, 4.67913934572691E-01, 9.49107912342759E-01,-
1 1.29484966168870E-01, 7.41531185599394E-01, 2.79705391489277E-01,-
1 4.05845151377397E-01, 3.81830050505119E-01,-0. E-00,-
1 4.17959183673469E-01, 9.60289856497536E-01, 1.01228536290376E-01,-
1 7.96666477413627E-01, 2.22381034453374E-01, 5.25532409916329E-01,-
1 3.13706645877887E-01, 1.83434642495650E-01, 3.6268378378362E-01,-
1 9.68160239507626E-01, 8.12743883615740E-02, 8.36031107326636E-01,-
1 1.80648160694857E-01, 6.13371432700590E-01, 2.60610696402935E-01,-
1 3.24253423403809E-01, 3.12347077040003E-01,-0. E-00,-
1 3.30239355001260E-01, 9.73906528517172E-01, 6.66713443086880E-02,-
1 8.65063366688985E-01, 1.49451349150581E-01, 6.79409568299024E-01,-
1 2.19086362515982E-01, 4.33395394129247E-01, 2.69266719309996E-01,-
1 1.48874338981631E-01, 2.95524224714753E-01/
DATA BB/-
1 9.78228658146057E-01, 5.56685671161740E-02, 8.87062599768095E-01,-
1 1.25580369464905E-01, 7.30152005574049E-01, 1.86290210927734E-01,-
1 5.19096129206812E-01, 2.33193764591990E-01, 2.69543155952345E-01,-
1 2.62804544510247E-01,-0. E-00,-
1 9.81560634246719E-01, 4.71753363865120E-02, 9.04117256370475E-01,-
1 1.06939325995318E-01, 7.69902674194305E-01, 1.60078328543346E-01,-
1 5.87317954286617E-01, 2.03167426723066E-01, 3.67831498998180E-01,-
1 2.33492536538355E-01, 1.25233408511469E-01, 2.49147045813403E-01,-
1 9.84183054718588E-01, 4.04840047653160E-02, 9.17598399222978E-01,-
1 9.21214998377280E-02, 8.01578090733310E-01, 1.38873510219787E-01,-
1 6.42349339440340E-01, 1.78145980761946E-01, 4.48492751036447E-01,-
1 2.07816047536889E-01, 2.30458315955135E-01, 2.26283180262897E-01,-
1-0. E-00,-
1 3.51194603317520E-02, 9.28434883663574E-01, 8.01580871597600E-02,-
1 8.27201315069765E-01, 1.21518570687903E-01, 6.87292904811685E-01,-
1 1.57203167158194E-01, 5.15248636358154E-01, 1.85538397477938E-01,-
1 3.19112368927890E-01, 2.05198463721296E-01, 1.08054948707344E-01,-
1 2.15263853463158E-01, 9.87992518020485E-01, 3.07532419961170E-02,-
1 9.372733924007C6E-01, 7.03660474881080E-02/
DATA CC/-
1 8.48206583410427E-01, 1.07159220467172E-01, 7.24417731360170E-01,-
1 1.39570677926154E-01, 5.70972172608539E-01, 1.66269205816994E-01,-
1 3.94151347077563E-01, 1.86161000015562E-01, 2.01194093997435E-01,-
1 1.98431485327112E-01,-0. E-00,-
1 9.89400934991650E-01, 2.71524594117540E-02, 2.02578241925561E-01,-
1 8.22535239386480E-02, 8.65631202387832E-01, 9.44575023073233E-01,-
1 7.554040408355003E-01, 1.24628971255534E-01, 6.17876244402644E-01,-
1 1.49595988816577E-01, 4.58016777657227E-01, 1.69156519395003E-01,-
1 2.81603550779259E-01, 1.82603415044924E-01, 9.50125098376370E-02,-
1 1.89450610455068E-01/
DO 50 I=1,70
J=2*I
JJ=2*I-1
A(I)=C(JJ)
H(I)=C(J)
50 CONTINUE
QUAD1 = 0.
IF (XI .EQ. XO) RETURN
N = NN
IF ( N .GT. 16) N=16
INDRT= MOD(N,2)+1
C INDRT = 1, N IS EVEN
C INDRT = 2, N IS ODD
GO TO (204,210),INDRT
204 MIN=(N*N)/4 -1
MAX=(N*(N+2))/4 -2
GO TO 215
210 MIN= (N*N-9)/4 +1
MAX= (N*(N+2)-11)/4
215 DELX=(XO-XI)/FLOAT(NS)
HDELX=.5*DELX
DO 260 K=1,NS
XA=FLOAT(K-1)*DELX + XI
DO 220 I=1,2
DO 220 J=MIN,MAX
A(J) = -A(J)
220 QUAD1 = QUAD1+H(J)*FGFK(XA+HDELX*(1.+A(J)))

```

```
      IF (INDKT .EQ. 2) QUAD1=QUAD1+H(MAX+1) *FOPX(XA+HDELX*(1.+A(MAX+1)))  
260  CCNTINUE  
      QUAD1 = HDELX*QUAD1  
270  RETURN  
      END
```

APPENDIX D

CALCULATION OF LIMITS OF INTEGRATION FOR NUMERICAL

EVALUATION OF NORMALIZED SHAPE FUNCTION

The integration indicated in equation (18) is performed numerically by replacing the infinite limits of integration and integrating the product $S_S(\nu, \nu')\psi(x, \Theta)$ over an interval where it is significant. Determination of practical limits involves finding an approximation for $\psi(x, \Theta)$ and for $S_S(\nu, \nu')\psi(x, \Theta)$. As these approximations involve products of Gaussian functions, it is necessary to find an expression for the product of two Gaussian functions.

Consider the two Gaussian functions $e^{-a(x-x_1)^2}$ and $e^{-b(x-x_2)^2}$ and their product

$$\exp[-a(x-x_1)^2] \exp[-b(x-x_2)^2] = \exp\left\{-[a(x-x_1)^2 + b(x-x_2)^2]\right\}$$

Expanding the exponent results in

$$\begin{aligned} a(x-x_1)^2 + b(x-x_2)^2 &= a(x^2 - 2xx_1 + x_1^2) + b(x^2 - 2xx_2 + x_2^2) \\ &= x^2(a+b) - 2x(ax_1 + bx_2) + ax_1^2 + bx_2^2 \end{aligned}$$

Completing the square in the first two terms gives

$$\begin{aligned} (a+b) \left[x^2 - 2x \frac{ax_1 + bx_2}{a+b} + \frac{(ax_1 + bx_2)^2}{(a+b)^2} \right] + ax_1^2 + bx_2^2 - \frac{(ax_1 + bx_2)^2}{a+b} \\ = (a+b) \left(x - \frac{ax_1 + bx_2}{a+b} \right)^2 + \frac{ab}{a+b} (x_1 - x_2)^2 \end{aligned}$$

and

$$\exp[-a(x-x_1)^2] \exp[-b(x-x_2)^2] = \exp\left[-\frac{ab}{a+b} (x_1 - x_2)^2\right] \exp\left[-(a+b) \left(x - \frac{ax_1 + bx_2}{a+b} \right)^2\right] \quad (D1)$$

The right side of equation (D1) is another Gaussian function, which has its maximum value $\exp \left\{ - \frac{[ab/(a+b)](x_1 - x_2)^2}{(a+b)^{-1/2}} \right\}$ at $x = (ax_1 + bx_2)/(a+b)$ and has a bandwidth proportional to $(a+b)^{-1/2}$.

The approximation of $\psi(x, \Theta)$ involves replacing S_R of equation (8) with

$$S_R = \frac{\beta}{\pi(\nu'' - \nu' + \beta^2)} \simeq \exp \left[- \frac{4 \ln 2}{4\beta^2} (\nu'' - \nu')^2 \right] = \exp \left[- \frac{4 \ln 2}{R_R^2} (\nu'' - \nu')^2 \right] \quad (D2)$$

The normalizing constants are discarded as only the functional behavior is now of concern.

The Lorenz-type Raman distribution is replaced by a Gaussian distribution having the same bandwidth. Then the Voigt function (eq. (9)) is approximately

$$S_V(\nu', \nu_j) \simeq \int_{-\infty}^{\infty} \exp \left[- \frac{4 \ln 2}{R_L^2} (\nu'' - \nu_j)^2 \right] \exp \left[- \frac{4 \ln 2}{R_R^2} (\nu'' - \nu')^2 \right] d\nu'' \quad (D3)$$

Using the results of equation (D1) gives

$$S_V(\nu', \nu_j) \simeq \exp \left[- \frac{4 \ln 2}{R_R^2 + R_L^2} (\nu' - \nu_j)^2 \right] \times \int_{-\infty}^{\infty} \exp \left[-4 \ln 2 \left(\frac{1}{R_R^2} + \frac{1}{R_L^2} \right) \left(\nu'' - \frac{R_R^2 \nu_j + R_L^2 \nu'}{R_R^2 + R_L^2} \right)^2 \right] d\nu'' \quad (D4)$$

This integral can be evaluated analytically. The result is

$$S_V(\nu', \nu_j) \propto \exp \left[- \frac{4 \ln 2}{R_R^2 + R_L^2} (\nu' - \nu_j)^2 \right] \quad (D5)$$

Equation (D5) would indicate that the Voigt bandwidth is given approximately by

$\sqrt{R_R^2 + R_L^2}$, but a better approximation is given in reference 15. It is

$$R_V = \frac{R_R}{2} + \sqrt{\left(\frac{R_R}{2} \right)^2 + R_L^2} \quad (D6)$$

Then

$$S_V(\nu', \nu_j) \propto \exp \left[- \frac{4 \ln 2}{R_V^2} (\nu' - \nu_j)^2 \right] \quad (D7)$$

and when equations (15) and (16) are used,

$$\psi(x, \Theta) \simeq \exp \left[- \frac{4 \ln 2}{R_V^2} (\nu' - \nu_j)^2 \right] \quad (D8)$$

This approximation to the first Doppler broadening integral gives an approximation to the shape function. Substituting (D8) in equation (18) yields

$$S(\nu, \nu_j) \simeq \int_{-\infty}^{\infty} \exp \left[- \frac{4 \ln 2}{R_S^2} (\nu' - \nu)^2 \right] \exp \left[- \frac{4 \ln 2}{R_V^2} (\nu' - \nu_j)^2 \right] d\nu' \quad (D9)$$

Again using equation (D1) results in

$$S(\nu, \nu_j) \simeq \exp \left[- \frac{4 \ln 2}{R_S^2 + R_V^2} (\nu - \nu_j)^2 \right] \times \int_{-\infty}^{\infty} \exp \left[-4 \ln 2 \left(\frac{1}{R_V^2} + \frac{1}{R_S^2} \right) \left(\nu' - \frac{R_V^2 \nu + R_S^2 \nu_j}{R_V^2 + R_S^2} \right)^2 \right] d\nu' \quad (D10)$$

At this point, it is possible to choose reasonable integration limits and use equation (18) to evaluate $S(\nu, \nu_j)$ numerically. Equation (D10) indicates that the integrand of equation (18) behaves roughly like a Gaussian function centered at

$$\nu' = \nu_C \simeq \frac{R_V^2 \nu + R_S^2 \nu_j}{R_V^2 + R_S^2} \quad (D11)$$

and with bandwidth

$$B_W \approx \left(\frac{1}{R_V^2} + \frac{1}{R_S^2} \right)^{-1/2} \quad (D12)$$

This information, together with the fact that

$$\int_{\nu_C - 3B_W}^{\nu_C + 3B_W} \exp \left[- \frac{4 \ln 2}{B_W^2} (\nu - \nu_C)^2 \right] d\nu = 0.999 \dots \int_{-\infty}^{\infty} \exp \left[- \frac{4 \ln 2}{B_W^2} (\nu - \nu_C)^2 \right] d\nu \quad (D13)$$

allows equation (18) to be replaced by

$$S(\nu, \nu_j) = \frac{1}{R_R} \int_{\nu_C - 3B_W}^{\nu_C + 3B_W} \exp \left[- \frac{4 \ln 2}{R_S^2} (\nu' - \nu)^2 \right] \psi(x, \Theta) d\nu' \quad (D14)$$

Equation (D14) is now in suitable form for integration by some standard technique, such as Simpson's rule or Gaussian quadratures (ref. 16). The latter technique is chosen because it gives the same results as a Simpson's rule method that uses step size control, but is much faster.

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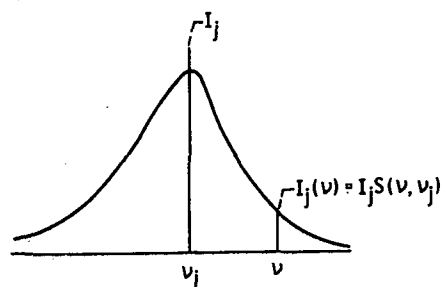


Figure 1. - Line broadening.

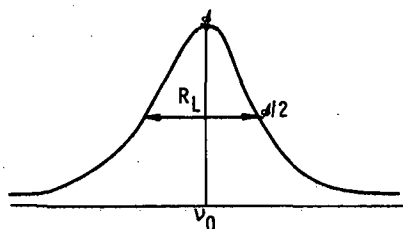


Figure 2. - Gaussian broadening function
 $S_L = \exp \left[(-4 \ln 2 / R_L^2) (\nu - \nu_0)^2 \right]$.

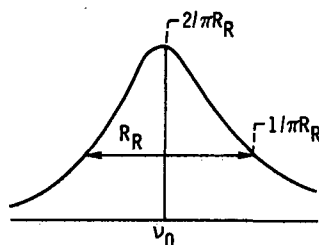


Figure 3. - Lorentz broadening function
 $S_R = (R_R / 2) / \pi \left[(\nu - \nu_0)^2 + (R_R / 2)^2 \right]$.

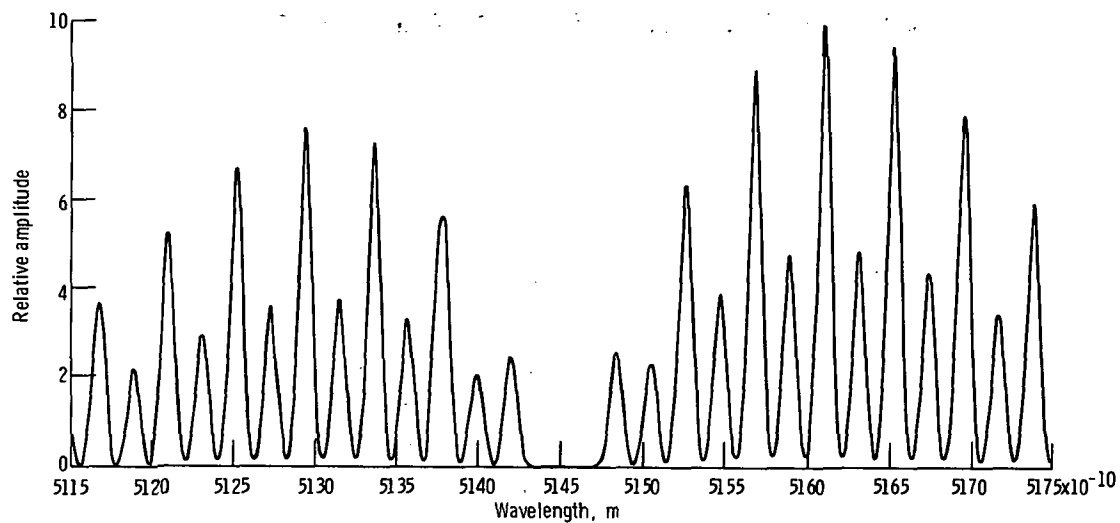


Figure 4. - Computed rotational Raman spectrum for N_2 at 300 K and 1 atmosphere.

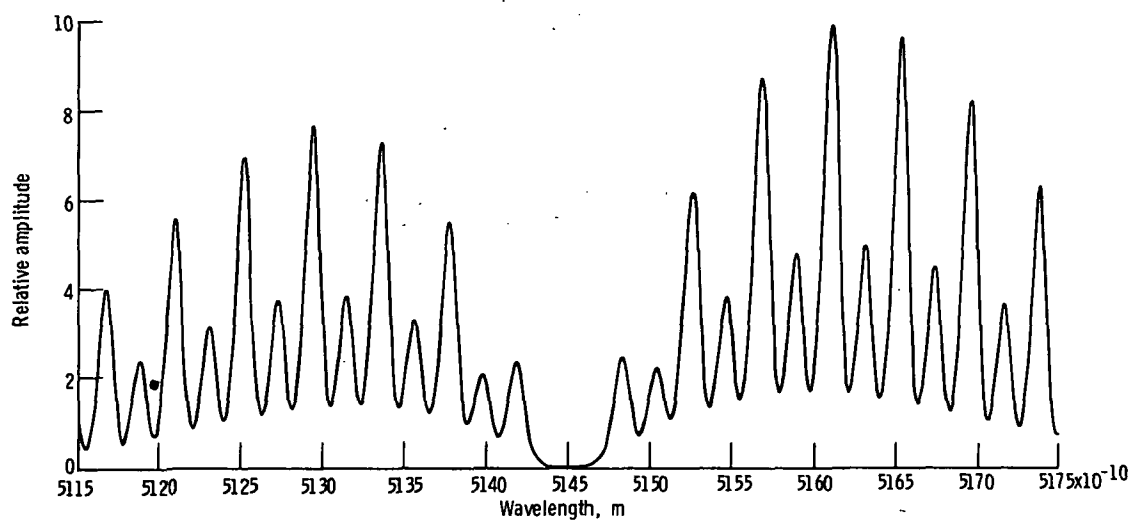


Figure 5. - Computed rotational Raman spectrum for N_2 at 300 K and 20 atmospheres.

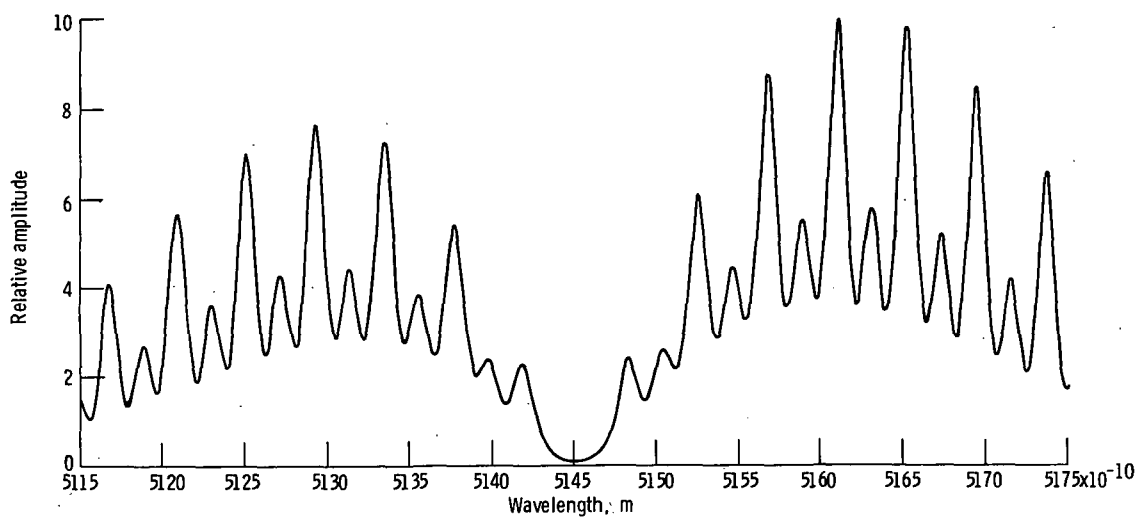


Figure 6. - Computed rotational Raman spectrum for N_2 at 300 K and 40 atmospheres.

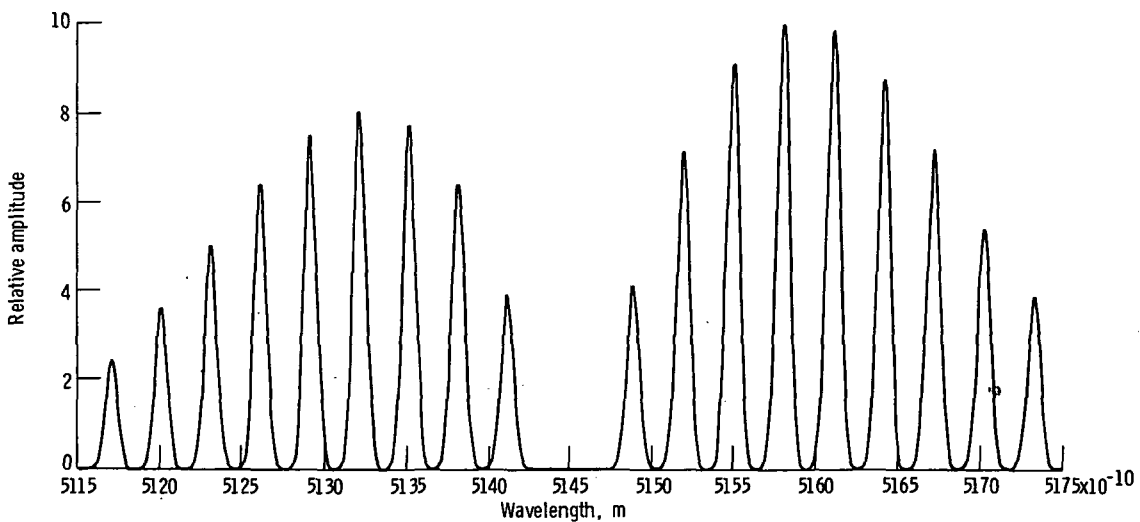


Figure 7. - Computed rotational Raman spectrum for O_2 at 300 K and 1 atmosphere.

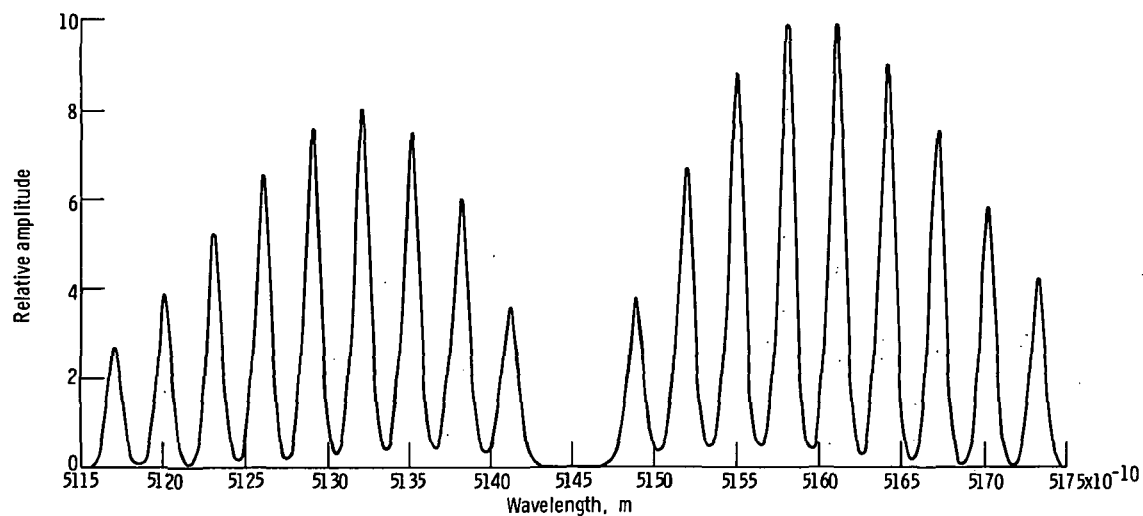


Figure 8. - Computed rotational Raman spectrum for O_2 at 300 K and 20 atmospheres.

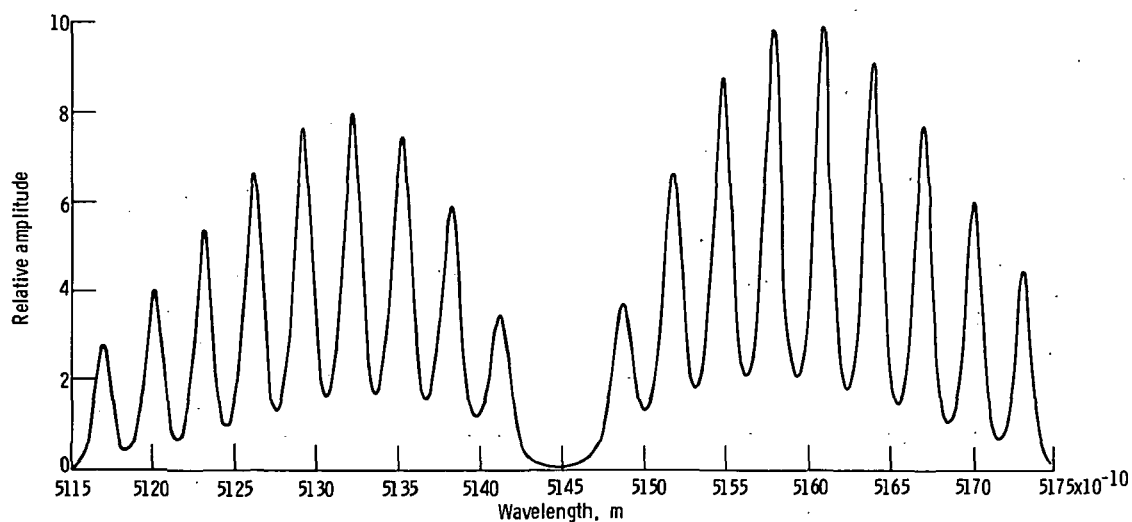


Figure 9. - Computed rotational Raman spectrum for O_2 at 300 K and 40 atmospheres.

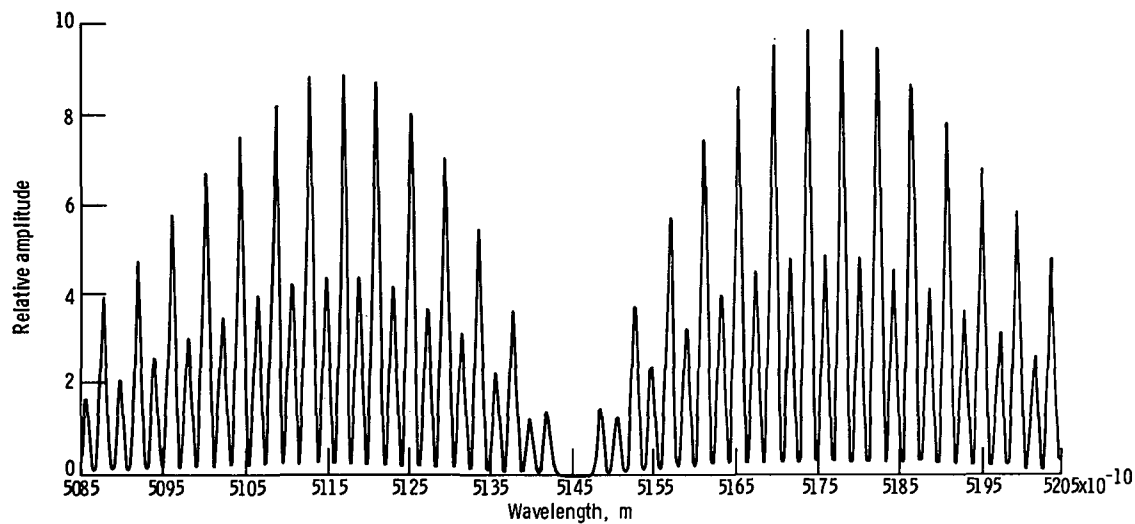


Figure 10. - Computed rotational Raman spectrum for N_2 at 1100 K and 1 atmosphere.

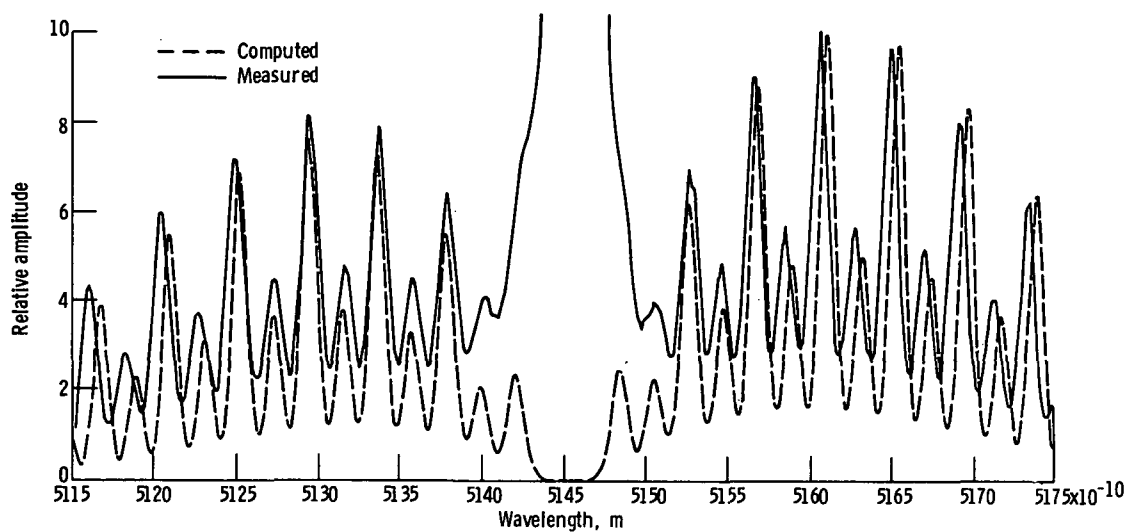


Figure 11. - Computed and measured Raman spectra for N_2 at 300 K and 19.4 atmospheres. For both curves, laser bandwidth, $0.166 \text{ centimeter}^{-1}$; slit bandwidth, $3.31 \text{ centimeter}^{-1}$; reciprocal of wave number of laser line, $5145 \times 10^{-10} \text{ meter}$ (5145 \AA).



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